

# A preliminary LCA case study: comparison of different pathways to produce purified terephthalic acid suitable for synthesis of 100 % bio-based PET

Yasuhiko Akanuma · Susan E. M. Selke · Rafael Auras

Received: 4 June 2013 / Accepted: 13 February 2014 / Published online: 25 February 2014  
© Springer-Verlag Berlin Heidelberg 2014

## Abstract

**Purpose** This study provides a preliminary comparison of the environmental burdens of three different pathways for production of bio-based purified terephthalic acid (PTA), suitable for the production of 100 % bio-based poly(ethylene terephthalate), PET. These pathways are through (1) muconic acid originating in wheat stover; (2) isobutanol originating in corn; and (3) benzene, toluene, and xylene (BTX) originating in poplar. The goal is to point out what areas of these processes are the largest environmental contributors and hence are the most critical for development of accurate primary data, as well as to indicate which of these pathways looks most promising, from an environmental viewpoint, for production of 100 % bio-based PET.

**Methods** Because much of the needed life cycle information to produce PTA is currently not available, inventory data for each scenario for the production of PTA were estimated based on the chemistry involved. In the impact analysis stage, the inventory data were classified and characterized with a focus on several environmental midpoint categories. SimaPro 7.3.3 software was used as the main computational software and Impact 2002+ v2.1 was used as the life cycle impact assessment methodology in this attributional life cycle assessment.

**Results and discussion** Valuable preliminary environmental impact data including identification of critical steps in the process were obtained. The global warming value of PET synthesized through the muconic acid scenario was 1.6 times larger than that of the scenario of PET synthesized through BTX even after a limited Monte Carlo simulation of 1,000 runs.

**Conclusions** Among the three scenarios for producing PET, PET synthesized through BTX looked the most promising to pursue for production of bio-based PET with lower environmental burdens. This work also indicated that the first production steps of producing PET through any of the evaluated scenarios (from biomass to the first intermediate) are responsible for the largest environmental burden and should be further characterized since they were the dominant processes in many impact categories.

**Keywords** Bio-based · Isobutanol · Muconic acid · Polyethylene terephthalate · Terephthalic acid · Toluene and xylene

## 1 Introduction

Life cycle assessment (LCA) is known as one of the most effective tools for evaluating the tradeoffs between environmental impacts and human activity. LCA can assess the environmental burdens for all life cycle stages of a product from material extraction to the factory gate (cradle to gate) or to final disposal and recycling (cradle to grave) (Handbook 2010). Interest in applying LCA has increased substantially, particularly in the packaging industry, due to recent sustainability initiatives and concerns (Dobon et al. 2011a, b). Each brand owner and/or producer of a product/package system must be responsible for managing the entire environmental burden of the production process (Lifset et al. 2013). Various approaches, including weight reduction and the use of

---

Responsible editor: Guido W. Sonnemann

**Electronic supplementary material** The online version of this article (doi:10.1007/s11367-014-0725-2) contains supplementary material, which is available to authorized users.

---

Y. Akanuma · S. E. M. Selke (✉) · R. Auras  
School of Packaging, Michigan State University, East Lansing,  
MI 48824-1223, USA  
e-mail: sselke@msu.edu

Y. Akanuma  
Suntory Business Expert Limited, Minato-ku,  
Tokyo 135-8631, Japan

recycled materials for packages, are used to reduce environmental burdens (Albrecht et al. 2013; Mirabella et al. 2013; Kang et al. 2013). Material used to produce the primary, secondary, and tertiary packaging systems and their end-of-life scenarios can have a large impact in the environmental footprint of product-package systems such as dairy milk (Eide 2002; González-García et al. 2012, bacon (Kang et al. 2013), seafood (Zufia and Arana 2008), strawberries (Madival et al. 2009), and the wine industry (Gazulla et al. 2010; Pattara et al. 2012).

Recently, some companies have tried to move from fossil-based resources to renewable resources for their products and production processes. Various bio-based polymeric packaging materials have been investigated and reported. Narayan et al. analyzed the LCA of starch-based polymers based on energy used for production, and compared the results with those of petrochemical-based polymers (Narayan and Patel 2003). Vink et al. focused on measuring the environmental sustainability and identifying environmental performance-improvement objectives for NatureWorks<sup>TM</sup> PLA (Vink et al. 2007). Kim and Dale estimated the environmental impact of polyhydroxybutyrate (PHB) derived from corn, and reported that it could reduce GHG emissions and energy consumption compared to petroleum-derived polymers (Kim and Dale 2008). Muska and Alles (2005) and Sunkara (2008) reported on 1,3-propanediol from corn as a feedstock chemical for polymers for various markets, including packaging, and Alles et al. (2010) discussed proper accounting for biogenic carbon in feedstock materials.

One of the most extensively used plastic packaging materials, especially for bottles and trays, is polyethylene terephthalate (PET) (Arena et al. 2003; Romero-Hernández et al. 2008; Shen et al. 2011; Foolmaun and Ramjeeawon 2012; Kuczenski and Geyer 2012). PET is synthesized by an esterification reaction between about 70 % by mass purified terephthalic acid (PTA) and about 30 % monoethylene glycol (MEG), with water as the byproduct of this polycondensation reaction. Conventionally, chemicals derived from petroleum resources are used to synthesize PET. Following the condensation polymerization, the molecular weight is increased by solid stating, in which the dried and crystallized resin chips from the original polymerization are subjected to high temperature and vacuum (Selke et al. 2004; Kang et al. 2011).

Production of MEG from renewable resources has already been accomplished by several material suppliers, enabling some brand owners to use bio-based PET, although no published LCA reports are available yet (Tuck et al. 2012). However, this limits the present bio-based PET bottle to about 30 % bio-based material. MEG is produced from ethylene by way of an intermediate substance (ethylene oxide). Ethylene can be produced through the dehydration of ethanol, or through the thermolysis of naphtha. For bio-based MEG, these C<sub>2</sub> containing compounds are made from cereal crops, sugar

crops or lignocellulosic biomass (Tuck et al. 2012). For the purposes of this study, bio-based MEG was modeled as made from corn as the feedstock.

Traditionally, PTA has been produced mainly by oxidation of para-xylene. Several companies are now developing bio-based PTA through various production methods, using glucose, sugar, lignocellulose, or algae as biomass resources (Tuck et al. 2012). There are three main pathways for future commercial production of bio-based PTA (Jong et al. 2012) utilizing (1) muconic acid; (2) isobutanol; or (3) benzene, toluene, and xylene (BTX) as the process intermediates. In this study, a preliminary LCA of producing 100 % bio-based PET resin was conducted using chemically based estimation of environmental life cycle inventory data, since actual process life cycle inventory (LCI) data is not available. Differing feedstocks were used in this preliminary study for the three chemical routes: wheat stover for the muconic acid pathway, sugar from corn for the isobutanol pathway, and poplar wood chips for the BTX pathway. The very limited data available, even for chemically based estimation, did not permit separation of the feedstock-specific inventory data from the inventory data for the initial process step.

Ideally, LCA comparisons between process alternatives are based on current data for commercial-scale processes. However, processes for production of bio-based PTA are not yet commercial, so this is not feasible. Because there are three distinct chemical pathways that are currently competing, and which are likely to have distinctly different environmental profiles, there is value in using chemically based estimation to provide a preliminary indication of which of these alternatives appear to be most promising from an environmental viewpoint. Additionally, such a study can help identify which parts of the production process appear to be the largest contributors to impacts of concern, so are most important to accurately characterize. Those are the aims of this study.

## 2 Methods

The goal of this initial LCA study was to compare the environmental burdens of bio-based PET resin with three different PTA production method scenarios: pathways through (1) muconic acid, (2) isobutanol, and (3) BTX as intermediates. Because this is a preliminary study, an important goal was to determine which pathway looks most promising from an environmental impact viewpoint, and what areas of the production process are large contributors and therefore are most important to accurately characterize. PET resin (1 kg) was chosen as the functional unit in this attributional cradle-to-gate study. Subsequent processes such as bottle blowing and assembly are identical to those used for petro-based PET, so were excluded from this study. SimaPro 7.3.3 software was used for modeling and computations.

In accordance with ISO 14044 requirements (ISO 14044, 2006), after the definition of system boundaries and objectives, data were collected in the LCI stage. Data sources included LCI databases, peer-reviewed literature, and patents. In a number of cases, no LCI data was available for some of the required processes, so estimations based on similar chemical reactions and material processes were used. In selection of appropriate benchmark processes, selection of the same chemical reaction process was given the highest priority, since the type of chemical production process, including its energy requirements and efficiency, is strongly related to the chemical reaction type. Material inputs were scaled in proportion to the relative reaction stoichiometry of the benchmark processes. Operational energies, however, were scaled in proportion to the mass of the output materials as the energy required to operate chemical production processes is typically much larger than the energy involved in the chemical reaction itself. Detailed LCI data calculation processes used in this study can be found elsewhere (Akanuma 2013) and are explained in further detail in the supporting materials available online.

Because of the preliminary nature of this study, in the life cycle impact assessment (LCIA) stage, the analysis was limited to the following indicators: global warming, terrestrial acidification/nitrification, aquatic acidification, aquatic eutrophication, nonrenewable energy, and mineral extraction. Global warming and nonrenewable energy were selected because of their importance and because collected data for these inventories is more robust than for many other impact categories. Mineral extraction, terrestrial acidification/nitrification, aquatic acidification, and aquatic eutrophication were chosen as these indicators are sensitive to differences between mineral- and bio-based production systems. Land use was not included due to lack of data. US LCI data was used where available, and the US electricity mix was used for all electrical energy. IMPACT 2002+ v2.1 (Jolliet et al. 2003) was selected as the LCIA method as it provides the selected midpoint indicators. Adding other LCIA methods can often provide useful insights, but was not considered warranted in this case, as a primary goal was to suggest areas for more detailed data development.

## 2.1 System boundaries

Figure 1 shows a summary of the products and processes considered for the purpose of this LCA study. The boxed arrows on the left indicate the manufacturing input. The arrows on the right stand for the outputs (including by-products). Although all emissions into the environment were included to the extent that data was available, the processes of capital equipment and maintenance, transportation of raw and processed materials, human labor, and other utilities, were excluded to concentrate on the production processes.

Since in some process steps, by-products are generated that are not used in later processes in this study, allocation was

based on generated mass ratios unless the data sources had already applied their own allocation rule. In such cases, the allocation rule already applied was maintained. For example, economic allocation was used for DDGS (dried distillers grains with solubles) in the “ethanol, 95 % in H<sub>2</sub>O, from corn, at distillery/US U” data from Ecoinvent v2.0.

## 2.2 Data and data quality requirements

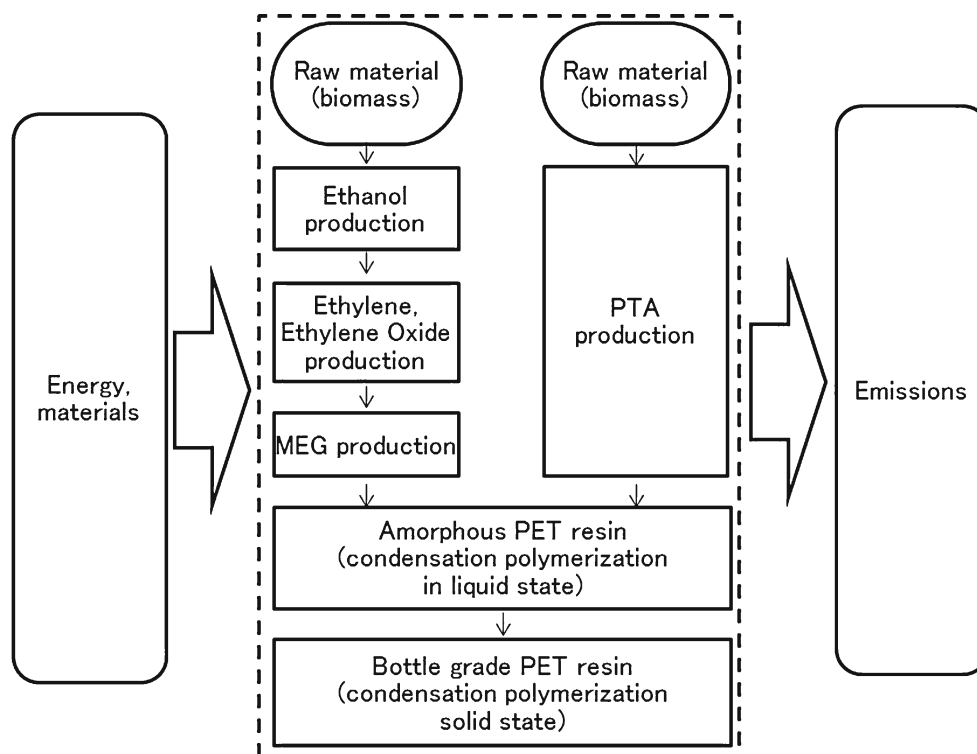
Data were obtained from the Ecoinvent v2.0, US-EI, and U.S. LCI databases. These data were from the past 10 years and based on current commercial scale operations. If non-US data were used, the US electricity mix was substituted. Some data was estimated from literature. In other cases, no specific inventory data was available so data were estimated based on information about related commercial scale processes (with the same or similar chemical reactions). Consistency and completeness checks for mass and energy balance results were conducted, and the quality of each dataset was evaluated with the use of a pedigree matrix. Details are discussed in the following section, with additional information in the [Electronic supplementary material](#) available online and in Akanuma (2013).

## 2.3 Material production

As shown in Fig. 2, three different scenarios were modeled for bio-based PTA production. These were coupled with one scenario for bio-based MEG production for production of bio-based PET.

### 2.3.1 PTA synthesis through the muconic acid pathway scenario

In this scenario, wheat stover (containing lignin) is the feedstock (Fig. 2). Lignin is an aromatic polymer that can be fermented to produce muconic acid. Since LCI data for this process are not available in databases, estimation was used. Van Duuren et al. (2011) provide an LCA from various raw materials to adipic acid. The adipic acid in this process was produced by hydrogenation of muconic acid under slightly elevated pressure (350 MPa). We assumed that the LCI data excluding the hydrogenation and later processes represents the LCI data for the raw material (wheat stover) to muconic acid stages. The obtained muconic acid is then converted into cyclohexa-2,5-diene-1,4-dicarboxylate using a Diels-Alder process (Burk et al. 2011). Muconic acid and acetylene are charged in a lab scale Parr reactor, and the reactor is then heated to 200 °C and held at this temperature for 12 h, at an initial pressure of 3.5 MPa (500 psi). Since no LCI data for this step were available, estimation was used based on the benchmark process of production of cyclohexane from benzene through a Diels-Alder reaction. Although acetylene can

**Fig. 1** PET resin system boundary

be produced from bio-based sources, no LCI data were found, so LCI data for petroleum-based acetylene were substituted.

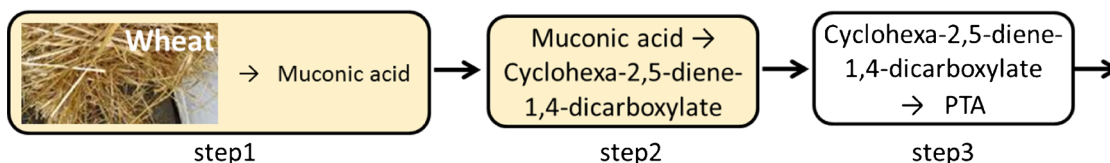
Cyclohexa-2,5-diene-1,4-dicarboxylate is then converted into TPA by dehydrogenation and purification. To estimate the LCI data, the process of dehydrogenation of xylene to TPA and its purification to PTA was used as the benchmark. Further

details are provided in the supporting material available online and in Akanuma (2013).

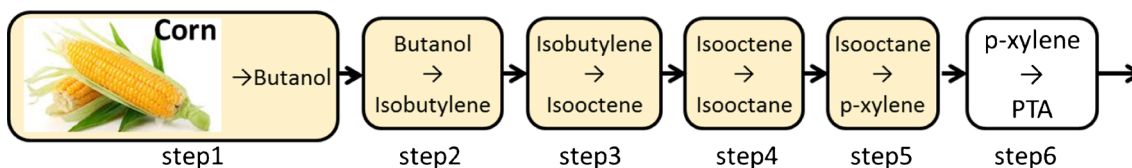
### 2.3.2 PTA synthesis through the isobutanol pathway scenario

In this scenario, raw material containing glucose from corn is the feedstock (Fig. 2). Specific yeasts, which produce bio-

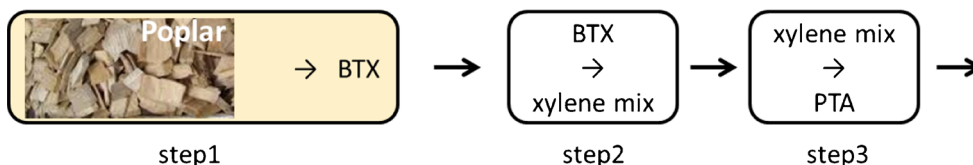
#### Scenario 1 (Muconic acid pathway)



#### Scenario 2 (Butanol pathway)



#### Scenario 3 (BTX pathway)

**Fig. 2** Schematic comparison of PTA production steps (*shaded* processes required estimation for their LCI data). “Wheat” refers to wheat stover



ethanol from a carbon source, can be modified to produce isobutanol via dry milling followed by fermentation (Feldman et al. 2011; Buelter et al. 2012). Since no LCI data were available for many of the steps for this pathway, it was necessary to estimate LCI data based on benchmark processes for many of these steps. Estimation for the initial glucose to isobutanol fermentation was based on fermentation of glucose to ethanol.

Isobutanol is then converted into isobutylene by dehydration. Dehydration of ethanol to ethylene, based on process data from Liptow et al. (2012), was used as the benchmark for this step. Isobutylene is then converted into isooctene by dimerization and hydrogenation; production of isooctene from C<sub>4</sub> components was used as the benchmark (Croezen et al. 2006, 2009). Isooctene is then converted into isooctane by hydrogenation; production of *n*-heptane from 1-heptene was used as the benchmark. Isooctane is then converted into para-xylene by dehydrocyclization; production of toluene from *n*-heptane was selected as the benchmark. Para-xylene is then converted into PTA by oxidation and purification; data was available from Ecoinvent for this step.

### 2.3.3 PTA synthesis through the BTX pathway scenario

In this scenario, bio-oil is produced from biomass (poplar) through fast pyrolysis in a CFB reactor (Iribarren et al. 2012). Next, catalytic upgrading with a zeolite catalyst is used to produce a BTX mix (Huber et al. 2006).

Extractive distillation of BTX produces a xylene mixture, which is converted into para-xylene by an adsorption, separation, and isomerization process. Para-xylene is converted into PTA by oxidation and purification. LCI data for BTX production were estimated from Iribarren et al. (2012). LCI data for extractive distillation of BTX were obtained assuming use of the sulfolane process (Meyers 2003). Data for the remaining steps were obtained from Ecoinvent.

### 2.3.4 MEG synthesis scenario

All three scenarios include the same MEG synthesis processes. The raw material, corn, is converted into C<sub>6</sub> sugar by fractionation and hydrolysis, and then converted to ethanol by fermentation. Ethanol is dehydrated into ethylene, and then oxidized and hydrated into MEG. Data for all process steps were obtained from Ecoinvent.

### 2.3.5 PET resin production

PET resin is obtained through condensation polymerization of MEG and PTA. The PET resin goes through additional polymerization in the solid state in order to increase its viscosity and yield bottle grade resin (Algeri and Rovaglio 2004). LCI data for all process steps were obtained from Ecoinvent.

## 3 Results and discussion

The IMPACT 2002+ V2.1 impact categories considered in this study were global warming, terrestrial acidification/nitrification, aquatic acidification, aquatic eutrophication, nonrenewable energy, and mineral extraction. Table 1 shows environmental impacts by process step for PET produced using each PTA pathway.

PTA production has the largest impact, for all PTA production scenarios, in the global warming, nonrenewable energy, terrestrial acidification/nitrification, aquatic acidification, and mineral extraction categories. For aquatic eutrophication, MEG production dominates in the muconic acid and BTX scenarios, but PTA production dominates in the isobutanol scenario. Production of corn, with associated irrigation and fertilization, is the primary contributor to aquatic eutrophication. In nearly all cases, step 1 of the PTA scenarios (the feedstock and initial chemical conversion step) is the largest contributor to the PTA impact. Step 3 in the BTX pathway, conversion of the xylene mix to PTA, has a larger impact than step 1 in the aquatic eutrophication and nonrenewable energy categories.

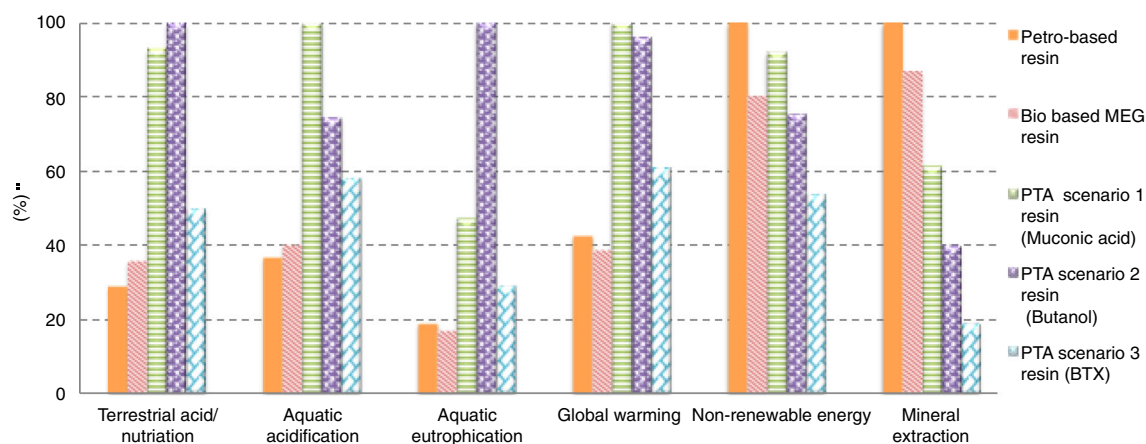
Figure 3 shows a comparison of the impact assessment results for the 3 100 % bio-based PET scenarios along with those for 100 % petro-based PET resin (using data from Ecoinvent v2.0 for MEG and PTA from petroleum resources) and PET from bio-based MEG and petro-based PTA. As a benchmark, the results from the 100 % petroleum-based PET resin scenario were compared with previous studies. The value for aquatic acidification was 13 g eq SO<sub>2</sub>, which is close to the literature value of 11 reported by Madival et al. (2009). The global warming value of 3,000 g eq CO<sub>2</sub> was very close to the value of 2,800 reported by Franklin Associates (2010).

The mineral extraction values for the 100 % bio-based resin scenarios were lower than those of petroleum-based resin, as expected. The BTX PTA scenario had the smallest mineral extraction values, followed by the butanol and muconic acid scenarios, in that order. For nonrenewable energy, the 100 % bio-based resins also had lower impact than the petroleum-based resin. The BTX and isobutanol scenarios had lower nonrenewable energy use than the partially bio-based PET, but the muconic acid-based PTA scenario had larger nonrenewable energy use. The feedstock transition from petroleum to bio-based appeared to increase, rather than reduce, the environmental impacts in the other categories. However, because the data used in this study depended heavily on estimation, it is premature to conclude that there are no benefits in these categories from the change in feedstock. Rather, the results show that such benefits cannot be assumed. Accurate data for production-scale processes is required before definitive conclusions can be drawn.

In all categories, the BTX scenario had lower impacts than the butanol and muconic acid scenarios. The butanol scenario

**Table 1** Summary of midpoint category values by process step for the production of PET resin. Process steps are described in Fig. 2

Impact category	Process step	Scenario 1 from wheat stover via muconic acid	Scenario 2 from corn via butanol	Scenario 3 from poplar via BTX
Terrestrial acidification/ nutrification kg SO <sub>2</sub> eq	MEG synthesis	2.95E-02	2.95E-02	2.95E-02
	PTA step 1	7.88E-02	8.21E-02	1.99E-02
	PTA step 2	7.30E-03	9.83E-03	2.41E-03
	PTA step 3	4.65E-03	1.88E-03	9.41E-03
	PTA step 4	—	6.39E-04	—
	PTA step 5	—	1.09E-03	—
	PTA step 6	—	4.65E-03	—
	PET synthesis	7.19E-03	7.19E-03	7.19E-03
	Total	1.27E-01	1.37E-01	6.84E-02
Aquatic acidification kg SO <sub>2</sub> eq	MEG synthesis	5.47E-03	5.47E-03	5.47E-03
	PTA step 1	2.28E-02	1.31E-02	7.32E-03
	PTA step 2	3.07E-03	1.87E-03	1.01E-03
	PTA step 3	1.16E-03	6.78E-04	3.84E-03
	PTA step 4	—	2.99E-04	—
	PTA step 5	—	9.04E-04	—
	PTA step 6	—	1.16E-03	—
	PET synthesis	2.81E-03	2.81E-03	2.81E-03
	Total	3.53E-02	2.62E-02	2.05E-02
Aquatic eutrophication kg PO <sub>4</sub> P-lim	MEG synthesis	8.09E-04	8.09E-04	8.09E-04
	PTA step 1	6.08E-04	2.29E-03	6.43E-06
	PTA step 2	3.92E-06	4.73E-05	1.14E-06
	PTA step 3	4.19E-05	6.91E-06	4.41E-05
	PTA step 4	—	3.37E-07	—
	PTA step 5	—	9.64E-07	—
	PTA step 6	—	4.19E-05	—
	PET synthesis	8.80E-05	8.80E-05	8.80E-05
	Total	1.55E-03	3.29E-03	9.48E-04
Global warming kg CO <sub>2</sub> eq	MEG synthesis	7.90E-01	7.90E-01	7.90E-01
	PTA step 1	4.85E+00	3.79E+00	2.07E+00
	PTA step 2	4.49E-01	6.71E-01	1.44E-01
	PTA step 3	3.74E-01	4.84E-01	6.76E-01
	PTA step 4	—	3.90E-02	—
	PTA step 5	—	2.46E-02	—
	PTA step 6	—	3.74E-01	—
	PET synthesis	6.33E-01	6.33E-01	6.33E-01
	Total	7.10E+00	6.81E+00	4.31E+00
Nonrenewable energy MJ primary energy	MEG synthesis	1.08E+01	1.08E+01	1.08E+01
	PTA step 1	4.58E+01	2.19E+01	1.14E+01
	PTA step 2	7.50E+00	8.31E+00	2.39E+00
	PTA step 3	6.94E+00	5.06E+00	1.23E+01
	PTA step 4	—	1.36E+00	—
	PTA step 5	—	1.93E+00	—
	PTA step 6	—	6.94E+00	—
	PET synthesis	1.09E+01	1.09E+01	1.09E+01
	Total	8.19E+01	6.72E+01	4.78E+01
Mineral extraction MJ surplus energy	MEG synthesis	5.83E-03	5.83E-03	5.83E-03
	PTA step 1	3.09E-02	1.69E-02	3.26E-03
	PTA step 2	1.00E-03	6.37E-04	2.88E-04
	PTA step 3	2.42E-03	2.27E-04	2.42E-03
	PTA step 4	—	6.33E-05	—
	PTA step 5	—	3.69E-05	—
	PTA step 6	—	2.42E-03	—
	PET synthesis	8.70E-04	8.70E-04	8.70E-04
	Total	4.11E-02	2.70E-02	1.27E-02



**Fig. 3** Comparison of LCIA results for PET production for the three PTA scenarios, petro-based PET, and partially bio-based PET (MEG bio, PTA petro)

had lower impacts than the muconic acid scenario for aquatic acidification, nonrenewable energy, and mineral extraction, but the muconic acid scenario had lower impacts in aquatic eutrophication. The butanol scenario had slightly lower impacts than muconic acid for global warming, and muconic acid for terrestrial acidification/nitrification, but these differences were judged too small to be significant.

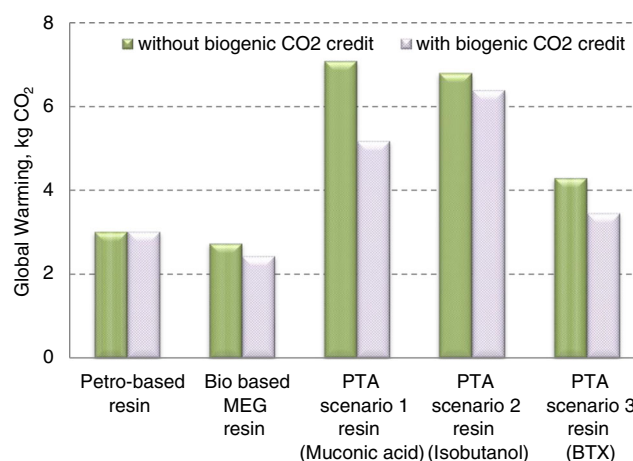
As discussed, wheat stover, corn, and poplar were the biomass sources for this study (Fig. 2). Production of PTA for 1 kg PET resin required 4.41 kg of wheat stover, 3.25 kg of corn, or 5.05 kg of poplar. Production of MEG for 1 kg of PET resin required 1.05 kg of corn. In the initial cradle-to-gate estimation using Impact 2002+, no credit was provided for CO<sub>2</sub> uptake for growing the bio-based feedstock materials. To examine this effect, an additional analysis was done assigning carbon credits by modifying the characterization factors for “CO<sub>2</sub>, in air” and “CO<sub>2</sub>, biogenic” in Impact 2002+ from “0 kg CO<sub>2</sub>-eq/kg” to “1 kg CO<sub>2</sub>-eq/kg.” (When the characterization factor is 0, no carbon credit is applied; a characterization factor of 1 applies the full amount of carbon uptake as a carbon credit.) The amount of CO<sub>2</sub> absorption for the muconic acid pathway was estimated using the carbon content of the muconic acid, as the available data did not allow us to separate biotic CO<sub>2</sub> from other operationally related CO<sub>2</sub>. For the butanol pathway, CO<sub>2</sub> uptake from the Ecoinvent corn inventory database was used. For the BTX pathway, literature values were used (Gonzalez-García et al. 2010). Figure 4 shows that the CO<sub>2</sub> credit reduced the global warming impact for the 100 % bio-based resins, as expected, but it still remained higher than for the petroleum-based and partially bio-based PET.

To further evaluate the robustness of the comparisons, the LCIA results were evaluated for data uncertainty using Monte Carlo simulation (1,000 runs). Details of the scores for the pedigree matrix are provided in the [Electronic supplementary material](#) available online. Figure 5 shows the results for global warming. Results were similar for the other categories. Standard deviations were calculated using a pedigree matrix

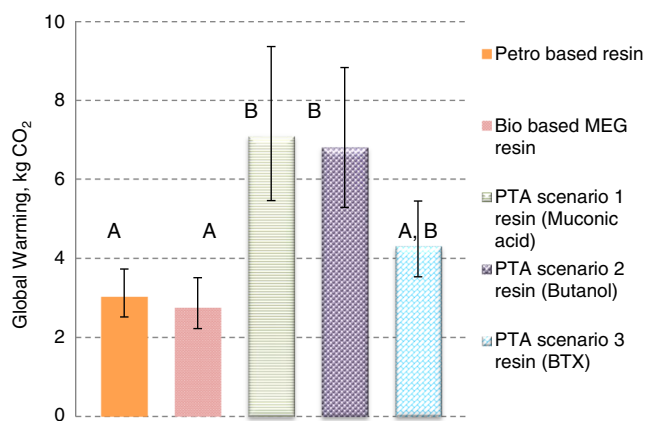
(available in [Electronic supplementary material](#) and in Akanuma 2013). These results suggest that the production of PET through the poplar to BTX pathway provides the most promising pathway of the three approaches examined for production of 100 % bio-based PET with reduced environmental burdens. However, caution must be used in judgments about the relative impacts of the differing PTA scenarios since they used different feedstocks. The initial PTA step dominated the impacts in most categories, and data available did not permit separation of the feedstock contributions from those of the first chemical conversion. Therefore, it was not possible to separate how much of the difference was due to the feedstocks and how much due to the chemical pathways.

#### 4 Conclusions

Selected environmental impacts of producing bio-based PET through three different bio-based PTA pathways (1) muconic acid beginning with wheat stover, (2) isobutanol beginning



**Fig. 4** Comparison of the results with/without biologically related CO<sub>2</sub> credit for the production of 1 kg PET resin



**Fig. 5** Impact results for global warming index including data variation among five scenarios (bars with different letters are statistically different  $P < 0.05$ )

with corn, and (3) BTX beginning with poplar chips were compared, using estimations for a number of processes for which no LCI data is available. Among the three scenarios, production of 100 % bio-based resin through the poplar-BTX pathway had the lowest estimated environmental impacts. For all the PTA scenarios, the first production step (from biomass to the 1<sup>st</sup> intermediate) usually was the largest contributor to the impacts. Since the biomass feedstocks used in this study differed, future research should focus on evaluating the impact of different bio-based materials that are suitable as feedstocks. For example, the use of agricultural by-products as biomass feedstocks might reduce the environmental burden significantly, which could reduce the environmental burden enough to be comparable to or smaller than the petroleum-based resin. Another important area is development of more accurate LCI data for the various processes involved. Ideally, data for state-of-the-art commercial scale operations would be used. This is obviously impossible when the various processes involved have not reached that state of development. As further research is done on development of bio-based PTA, LCI data should be collected for these processes, so it can be used to better compare the environmental profiles of these alternatives. As discussed in Hetherington et al. (2014), there are good reasons to use LCA as a guide during efforts to develop products and processes with reduced environmental impacts.

Another issue that should be addressed is the consequences of further use of biomass sources for production of PET. The effects of changing land use, in particular, are increasingly being examined in consequential LCAs-CLCA (e.g. Hertel et al. 2010; Searchinger et al. 2008). The whole field of consequential LCA is of increasing interest (e.g. Vázquez-Rowe et al. 2013). While this study is confined to the attributional approach, CLCA needs to be used to inform the larger discussion of increased use of bio-based feedstocks for commodity plastics.

**Acknowledgement** The authors would like to thank Satish Joshi for insightful comments and suggestions regarding the original work, and SUNTORY for financially supporting and sponsoring Y. Akanuma through his MS degree.

## References

- Akanuma Y (2013) LCA comparison of 100 % bio-based PET synthesized from different PTA pathways. M.S. Thesis, Michigan State University. Available from ProQuest, UMI Dissertations Publishing, AAT 1536872
- Albrecht S, Brandstetter P, Beck T, Fullana-i-Palmer P, Grönman K, Baitz M, Deimling S, Sandilands J, Fischer M (2013) An extended life cycle analysis of packaging systems for fruit and vegetable transport in Europe. *Int J Life Cycle Assess* 18(8):1549–1567
- Algeri C, Rovaglio M (2004) Dynamic modeling of a poly(ethylene terephthalate) solid-state polymerization reactor I: detailed model development. *Ind Eng Chem Res* 43(15):4253–4266
- Alles C, Ginn J, Veith S (2010) GHG inventory of bio-based Sorona® polymers. LCA X, Portland, OR. <http://www.lcaxcenter.org/LCAX/presentations-final/265.pdf>. Accessed 19 Aug 2013
- Arena U, Mastellone ML, Perugini F (2003) Life cycle assessment of a plastic packaging recycling system. *Int J Life Cycle Assess* 8(2):92–98
- Buelter T et al. (2012) Reduced by-product accumulation for improved production of isobutanol. US. 8,133,715 B2
- Burk MJ, Osterhout RE, Sun J (2011) Semi-synthetic terephthalic acid via microorganisms that produce muconic acid. US. 2011/0124911 A1
- Croezen H et al. (2006) ETBE and ethanol: a comparison of CO<sub>2</sub> savings. CE Delft. [http://www.ce.nl/publicatie/etbe\\_and\\_ethanol%3A\\_a\\_comparison\\_of\\_co2\\_savings/715](http://www.ce.nl/publicatie/etbe_and_ethanol%3A_a_comparison_of_co2_savings/715). Accessed 29 Jan 2013
- Croezen H et al (2009) The impact of ethanol and ETBE blending on refinery operations and GHG-emissions. *Energy Pol* 37(12):5226–5238
- Dobon A et al (2011a) The sustainability of communicative packaging concepts in the food supply chain. A case study: part 1. Life cycle assessment. *Int J Life Cycle Assess* 16(2):168–177
- Dobon A et al (2011b) The sustainability of communicative packaging concepts in the food supply chain. A case study: part 2. Life cycle costing and sustainability assessment. *Int J Life Cycle Assess* 16: 537–547
- Eide M (2002) Life cycle assessment (LCA) of industrial milk production. *Int J Life Cycle Assess* 7:115–126
- Feldman R et al. (2011) Yeast organism producing isobutanol at a high yield. US. 8,017,375 B2
- Foolmaun R, Ramjeeawon T (2012) Comparative life cycle assessment and social life cycle assessment of used polyethylene terephthalate (PET) bottles in Mauritius. *Int J Life Cycle Assess* 18(1):155–171
- Franklin Associates (2010) Final report, Cradle-to-gate life cycle inventory of nine plastic resins and four polyurethane precursors. [http://www51.honeywell.com/sm/chemicals/enovate/common/documents/FP\\_Enovate\\_July\\_2010\\_Report\\_by\\_the\\_American\\_Chemistry\\_Council\\_Manual.pdf](http://www51.honeywell.com/sm/chemicals/enovate/common/documents/FP_Enovate_July_2010_Report_by_the_American_Chemistry_Council_Manual.pdf). Accessed 25 Feb 2013
- Gazulla C, Raugel M, Fullana-i-Palmer P (2010) Taking a life cycle look at crianza wine production in Spain: where are the bottlenecks? *Int J Life Cycle Assess* 14:330–337
- Gonzalez-García S, Gasol C, Gabarrell X, Rieradevall J, Moreira M, Feijoo G (2010) Environmental profile of ethanol from poplar biomass as transport fuel in Southern Europe. *Renew Energy* 35: 1014–1023
- González-García S, Castanheira ÉG, Dias AC, Arroja L (2012) Environmental life cycle assessment of a dairy product: the yoghurt. *Int J Life Cycle Assess* 18:796–811
- Handbook ILCD (2010) General guide for the life cycle assessment—detailed guidance. Luxembourg. doi:10.2788/38479



- Hertel T, Golub A, Jones A, O'Hare M, Plevin R, Kammen D (2010) Effects of US maize ethanol on global land use and greenhouse gas emissions: estimating market-mediated responses. *Bioscience* 60:223–231
- Hetherington A, Borrión A, Griffiths O, McManus M (2014) Use of LCA as a development tool within early research: challenges and issues across different sectors. *Int J Life Cycle Assess* 19(1):130–143
- Huber G, Iborra S, Corma A (2006) Synthesis of transportation fuels from biomass: chemistry, catalysts, and engineering. *Chem Rev* 106:4044–4098
- Iribarren D, Peters J, Dufour J (2012) Life cycle assessment of transportation fuels from biomass pyrolysis. *Fuel* 97:812–821
- Joliet O, Margni M, Charles R, Humbert S, Payet J, Rebitzer J, Rosenbaum R (2003) IMPACT 2002+: a new life cycle impact assessment methodology. *Int J Life Cycle Assess* 8(6):324–330
- Jong ED, Higson A, Walsh P, Wellisch M (2012) Bio-based chemical—value added products from biorefineries. The IEA Bioenergy Rep. <http://www.ieabioenergy.com/Download.aspx?DocId=7312>. Accessed 25 Feb 2013
- Kang DH, Auras R, Vorst K, Singh J (2011) An exploratory model for predicting post-consumer recycled PET content in PET sheets. *Poly Test* 30(1):60–68
- Kang D, Sgriccia N, Selke S, Auras R (2013) Comparison of bacon packaging on a life cycle basis: a case study. *J Clean Prod* 54:142–149
- Kim S, Dale B (2008) Energy and greenhouse gas profiles of polyhydroxybutyrate derived from corn grain: a life cycle perspective. *Environ Sci Technol* 42:7690–7695
- Kuczenski B, Geyer R (2012) PET bottle reverse logistics—environmental performance of California's CRV program. *Int J Life Cycle Assess* 18(2):456–471
- Lifset R, Atasu A, Tojo N (2013) Extended producer responsibility-national, international, and practical perspectives. *J Ind Ecol* 17(2):162–166
- Liptow C, Tillman A (2012) Comparative life cycle assessment of polyethylene based on sugarcane and crude oil. *J Ind Ecol* 16(3):420–435
- Madival S, Auras R, Singh S, Narayan R (2009) Assessment of the environmental profile of PLA, PET and PS clamshell containers using LCA methodology. *J Clean Prod* 17:1183–1194
- Meyers R (2003) Handbook of petroleum refining processes, 3<sup>rd</sup> ed, McGraw Hill, chapter 9
- Mirabella N, Castellani V, Sala S (2013) Life cycle assessment of bio-based products: a disposable diaper case study. *Int J Life Cycle Assess* 18(5):1036–1047
- Muska C, Alles C (2005) Biobased 1,3-propanediol, a new platform chemical for the 21st century, *BioPerspectives* 2005. <http://brew.geo.uu.nl/BREWsymposiumWiesbaden11mei2005/WEBSITEBrewPresentations51105.PDF>. Accessed 20 Aug 2013
- Narayan R, Patel M (2003) Review and analysis of bio-based product LCAs. <http://www3.abe.iastate.edu/biobased/lcareview.pdf>. Accessed 29 Jan 2013
- Pattara C, Raggi A, Cichelli A (2012) Life cycle assessment and carbon footprint in the wine supply-chain. *Env. Mgt* 49:1247–1258
- Romero-Hernández O, Romero Hernández S, Muñoz D, Detta-Silveira E, Palacios-Brun A, Laguna A (2008) Environmental implications and market analysis of soft drink packaging systems in Mexico. A waste management approach. *Int J Life Cycle Assess* 14(2):107–113
- Searchinger T, Heimlich R, Houghton R, Dong F, Elobeid A, Fabiosa J, Tokgoz S, Hayes D, Yu T (2008) Use of U.S. croplands for biofuels increases greenhouse gases through emissions from land-use change. *Science* 319:1238–1240
- Selke S, Culter J, Hernández R (2004) Plastic packaging—property, processing, application and regulations, 2nd edn. Hanser, Cincinnati
- Shen L, Nieuwlaar E, Worrell E, Patel M (2011) Life cycle energy and GHG emissions of PET recycling: change-oriented effects. *Int J Life Cycle Assess* 16(6):522–536
- Sunkara H (2008) DuPont<sup>RM</sup> Cerenol<sup>TM</sup>: a new family of sustainable and environmentally friendly materials. 12th Annual Green Chemistry and Engineering Conference, Washington, DC
- Tuck C, Perez E, Horvath I, Sheldon R, Poliakov M (2012) Valorization of biomass: deriving more value from waste. *Science* 337:695–699
- Van Duuren J, Brehmer B, Mars A, Eggink G, Martins dos Santos V, Sanders J (2011) A limited LCA of bio-adipic acid: manufacturing the nylon-6,6 precursor adipic acid using the benzoic acid degradation pathway from different feedstocks. *Biotechnol Bioeng* 108:1298–1306
- Vázquez-Rowe I, Rege S, Marvuglia A, Thénie J, Haurie A, Benetto E (2013) Application of three independent consequential LCA approaches to the agricultural sector in Luxembourg. *Int J Life Cycle Assess* 18:1593–1604
- Vink E, Glassner D, Kolstad J, Wooley R, O'Connor (2007) The eco-profiles for current and near-future NatureWorks<sup>®</sup> polylactide (PLA) production. *Ind Biotechnol* 3:58–81
- Zufia J, Arana L (2008) Life cycle assessment to eco-design food products: industrial cooked dish case study. *J Clean Prod* 16:1915–1921